Quantum Coulomb glass – Hartree-Fock approximation versus exact diagonalization

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(February 7, 2008)

We investigate the behavior of disordered interacting electrons in the insulating regime. Our study is based on the quantum Coulomb glass model which is obtained from the classical Coulomb glass by adding hopping matrix elements between neighboring sites. We use two different numerical methods, viz. a Hartree-Fock approximation and an exact diagonalization and compare the results for the tunneling density of states and the localization properties in order to determine the range of validity of the Hartree-Fock method. We find that the Hartree-Fock method gives a good approximation for the density of states for all energies but represents the localization properties correctly close to the Fermi level only. Some consequences for the localization of disordered interacting electrons are discussed.

71.55.Jv, 72.15.Rn, 71.30.+h

The physics of disordered interacting electrons has been a subject of great interest within the last two decades. Most work, both experimental and theoretical has concentrated on the metallic regime where experiments are easier to carry out and theoretical studies can be based on established perturbative methods [1]. In comparison, the insulating regime has seen much less activities. Experimentally, this is due to the fact that transport properties vanish in an insulator at zero temperature. On the theoretical side, the main reason is that perturbative methods cannot be applied since the insulating (classical) limit [2,3] itself is a complicated many-particle problem. The prototype model in the classical insulating regime is the Coulomb glass model [4] which describes the electrons as classical point charges.

Recently, the attention has focused on the quantum insulating regime closer to the metal-insulator transition (MIT) where the description in terms of classical point charges becomes questionable. These new studies try to address two main problems: (i) one wants to gain an understanding of the MIT itself by approaching it from the insulating side which is complementary to the usual approach based on perturbation theory around the metallic system; (ii) one wants to know whether the key properties of the insulating limit as, e.g., the Coulomb gap in the single-particle density of states (DOS) [3], carry over to the regime close to the MIT where most of the experiments on insulators are performed.

The prototype model for the quantum insulating regime is the quantum Coulomb glass model [5–7]. It is defined on a regular hypercubic lattice with $N = L^d$ (d is the spatial dimensionality) sites occupied by KN (spinless) electrons ($0 < K < 1$). To ensure charge neutrality each lattice site carries a compensating positive charge of Ke. The Hamiltonian of the quantum Coulomb glass is obtained from the classical Coulomb glass by adding hopping terms of strength t between nearest neighbor sites. It reads

$$H = -t\sum_{\langle ij\rangle}(c_i^\dagger c_j + c_j^\dagger c_i) + \sum_i(\varphi_i - \mu)n_i + \frac{1}{2}\sum_{i\neq j}(n_i - K)(n_j - K)U_{ij} \quad (1)$$

where $c_i^\dagger$ and c_i are the electron creation and annihilation operators at site i, respectively, and $\langle ij\rangle$ denotes all pairs of nearest neighbor sites. n_i is the occupation number of site i and μ is the chemical potential. The Coulomb interaction $U_{ij} = e^2/r_{ij}$ remains long-ranged since screening breaks down in the insulating phase. The random potential values φ_i are chosen independently from a box distribution of width $2W_0$ and zero mean.

In a previous paper [5] we have investigated the quantum Coulomb glass by means of a Hartree-Fock (HF) approximation. Within this method the interaction was treated at HF level and the arising self-consistent disordered single-particle problem was diagonalized numerically. This method enabled us to study comparatively large systems of up to 10^3 sites and a large number of different disorder configurations. We found that the Coulomb gap persists in the entire insulating phase but becomes narrower when approaching the MIT. The depletion of the DOS in turn leads to an enhancement of localization close to the Fermi level. This enhancement seems to be in contradiction to the results of Talamantes et al. [7] who inferred an interaction-induced delocalization from an investigation of the many-particle spectrum. Since the HF method is a severe approximation it is not clear whether the seeming disagreement is an artificial result of the HF approximation or whether it can be attributed to the use of different criteria [6] for localization in a many-particle system or being in a different part of parameter space.

In this paper we therefore investigate the range of va-

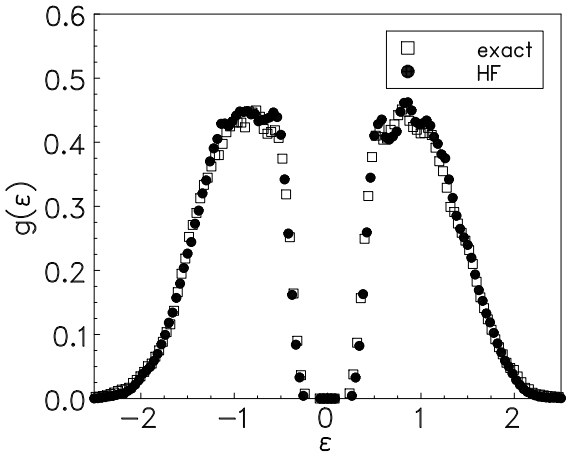

FIG. 1. Comparison of the exact and Hartree-Fock results for the single-particle DOS of a quantum Coulomb glass with 3x4 sites for $W_0 = 1$, $K = 0.5$ and $t = 0.1$. The data represent averages over 1600 different disorder configurations.

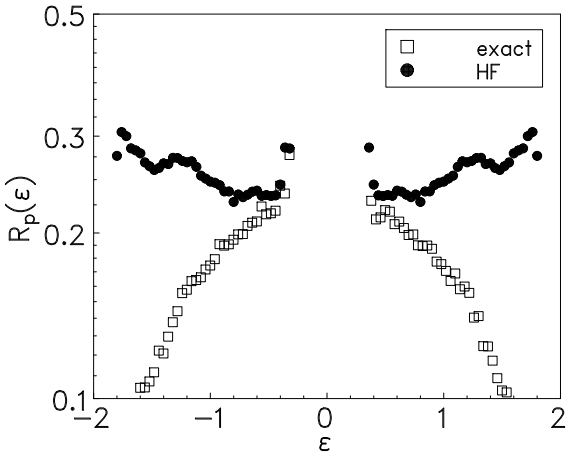

FIG. 2. Comparison of the Hartree-Fock and exact results for the return probability R_p for a particle in a quantum Coulomb glass with 3x4 sites for $W_0 = 1$, $K = 0.5$ and $t = 0.3$. The data represent averages over 1600 different disorder configurations.

lidity of the HF approximation by comparing it to the results of numerically exact diagonalization of small lattices with up to 16 sites.

We first discuss the single-particle (i.e. tunneling) DOS $g(\varepsilon)$. In a many-particle system in general the DOS is defined via the single-particle Greens function

$$g(\varepsilon) = -\frac{1}{\pi}\,\mathrm{Im}\,\mathrm{tr}\,G^R(\varepsilon). \tag{2}$$

Within the HF approximation the single-particle energies are simply given by the eigenvalues of the HF Hamiltonian. A comparison of the single-particle DOS resulting from the HF and exact calculations for one particular set of parameters in Fig. 1 shows good agreement. We have performed analogous calculations for different values of the overlap ($t = 0 \ldots 0.8$) and filling factors ($K = 0.5$ and 0.25). For all parameter sets investigated we found that the results of both methods agree within the statistical errors. Thus we conclude that the single-particle DOS of the quantum Coulomb glass is well described within the HF approximation. We note, however, that we cannot make a statement about the validity of the HF approximation asymptotically close to the Fermi energy since the small systems which we can study by exact diagonalization always possess a sizeable hard gap which obscures the Coulomb gap.

We now turn to the localization properties. The simplest measure of localization for a single-particle state $|\psi_\nu\rangle$ in a non-interacting system is the inverse participation number

$$P_\nu^{-1} = \sum_j |\langle\psi_\nu|j\rangle|^4 \tag{3}$$

where the sum runs over all sites j. In practice it is often averaged over all states with a certain energy ε

$$P^{-1}(\varepsilon) = \frac{1}{g(\varepsilon)}\,\frac{1}{N}\sum_\nu P_\nu^{-1}\,\delta(\varepsilon - \varepsilon_\nu)\ . \tag{4}$$

The generalization of the participation number to many-particle systems is not straightforward, for a discussion see e.g. Ref. [6]. A consistent generalization of P^{-1} is the probability R_p for a particle to return to its starting site in infinite time, which can be expressed in terms of single-particle Greens functions

$$R_p(\varepsilon) = \frac{1}{N}\sum_j \lim_{\delta\to 0}\frac{\delta}{\pi}\,G_{jj}(\varepsilon + i\delta)\,G_{jj}(\varepsilon - i\delta). \tag{5}$$

For non-interacting electrons $P^{-1}(\varepsilon) = R_p(\varepsilon)$. In Fig. 2 we compare the return probability obtained by Hartree-Fock and exact calculations. Close to the Fermi energy the HF and exact results agree reasonably well. Away from the Fermi energy the return probability obtained by exact diagonalization decreases drastically which is not correctly described by HF [8]. We have carried out analogous calculations for different values of overlap ($t = 0 \ldots 0.8$) and filling factors ($K = 0.5$ and 0.25). For all parameter sets we found the same behavior, viz. the HF method overestimates the return probability away from the Fermi energy whereas both methods agree close to the Fermi level.

To summarize, we have compared the results of a HF approximation and of an exact diagonalization of the quantum Coulomb glass. We found that the results of the two methods for the DOS agree reasonably well for all energies. The localization properties are correctly described by HF close to the Fermi energy only. In particular, the interaction-induced enhancement of localization which we found [5] within the HF approximation is also present in the exact calculation. Consequently, it

appears that the seeming contradiction between the HF calculation [5] and Ref. [7] is not an artefact of the HF approximation but either due to the use of *different quantities* to characterize localization in a many-body system or due to being in *different parts* of parameter space. Thus a detailed investigation of the different localization criteria seems to be necessary [6]. The results of the present paper not only justify the application of the HF method to analyze at least some properties of the quantum Coulomb glass (taking into account the fact that the relevant physics at low temperatures is dominated by excitations close to the Fermi energy), they also suggest an improved calculational scheme. It consists of two steps: (i) solving the model within HF approximation and (ii) expanding the many-particle states in an energetically cutoff HF basis and diagonalizing this reduced problem. Such a scheme will enable us to treat comparatively large lattices and still obtain almost exact results for energies close to the Fermi energy. Work along these lines is in progress.

This work was supported in part by the DFG under grant nos. Schr231/13-1, Vo659/1-1 and SFB393 and by the NSF under grant no. DMR-95-10185.

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